

Generalized Pyrolysis Model for Combustible Solids

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Motivation – Big Picture



- Reliable prediction of large-scale fire development
- Predictive capabilities for solid-phase pyrolysis lags gas-phase
 - “Practical” or “real-world” materials poorly understood
 - Many models specific to one class of materials





Objectives



- 1) Develop generalized pyrolysis model
 - Thermoplastic, charring, intumescent, smolder
 - Practical/real-world materials

- 2) Develop technique to estimate model input parameters from existing laboratory tests
 - Fire tests (Cone Calorimeter, FPA)
 - Thermal analysis (TGA, DSC)



Presentation Outline



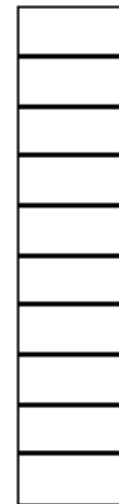
- Motivation
- Objectives
- Generalized pyrolysis model description
- Generalized pyrolysis model application
 - Oxidative pyrolysis of white pine
 - Thermal pyrolysis of polypropylene
 - Heating and swelling of intumescent coating
- Concluding remarks



Generalized Pyrolysis Model



- Decomposing solid treated as coupled gaseous and condensed phases
- 1D conservation equations solved for
 - Gas and solid mass
 - Gas and solid species
 - Gas and solid energy
 - Gas momentum (Darcy's law)
- Volume change handled by variable grid spacing



Surface regression



Generalized Pyrolysis Model



- User may specify any number of
 - Distinct layers
 - Solid and gaseous species
 - Solid and gaseous reactions

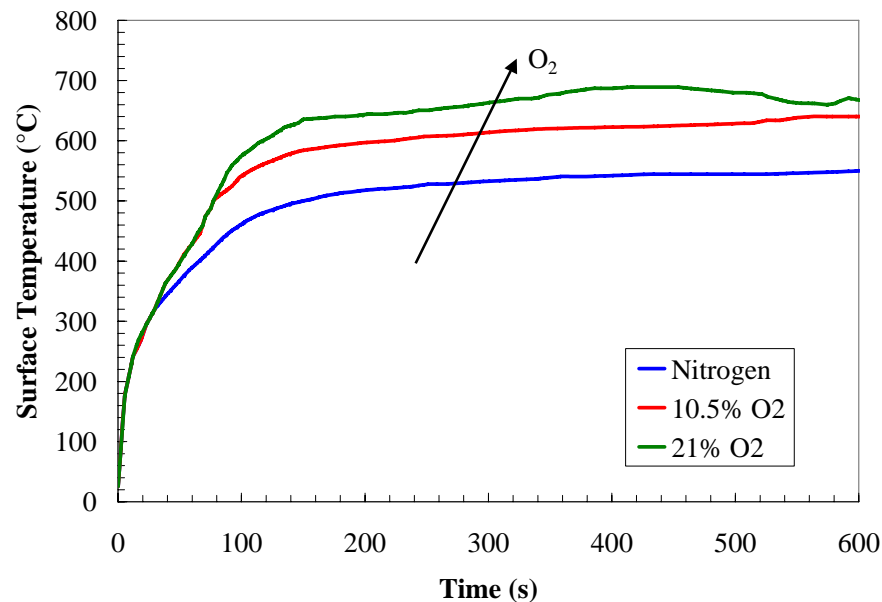
- Physics include
 - Volume change (swelling/surface regression)
 - In-depth radiation absorption, radiative transfer across pores
 - Darcy flow through porous media (pressure solver)
 - Penetration of ambient oxygen into decomposing solid and its effect on gaseous and solid reactions



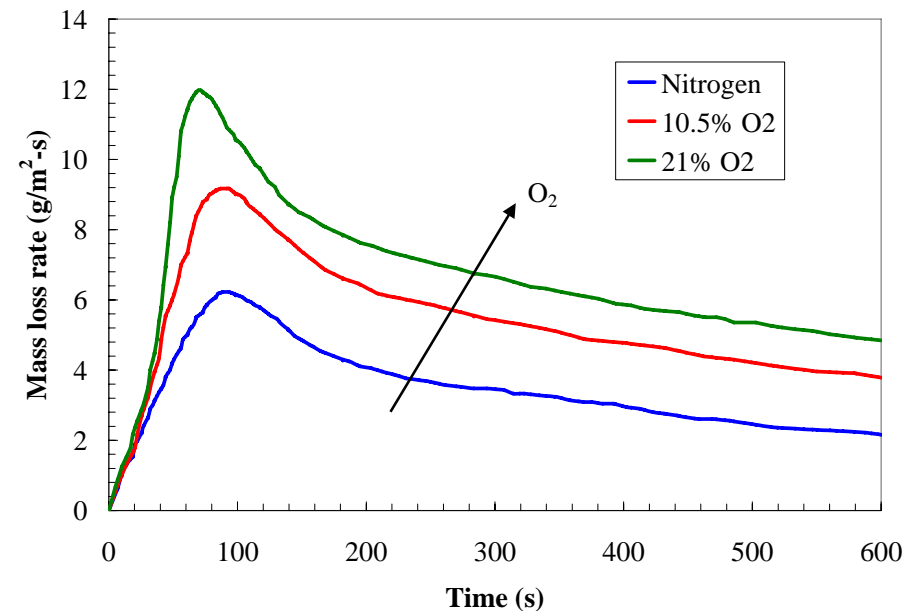
White Pine Oxidative Pyrolysis – Experimental Data



- Ohlemiller, Kashiwagi, Werner - *C+F* v69 (1987)
 - 3.8 cm cubes irradiated @ 40 kW/m² (natural convection)
 - O₂ ranged from 0% to 21% by volume



Surface temperature



Mass loss rate



White Pine Oxidative Pyrolysis – Numerical Simulation



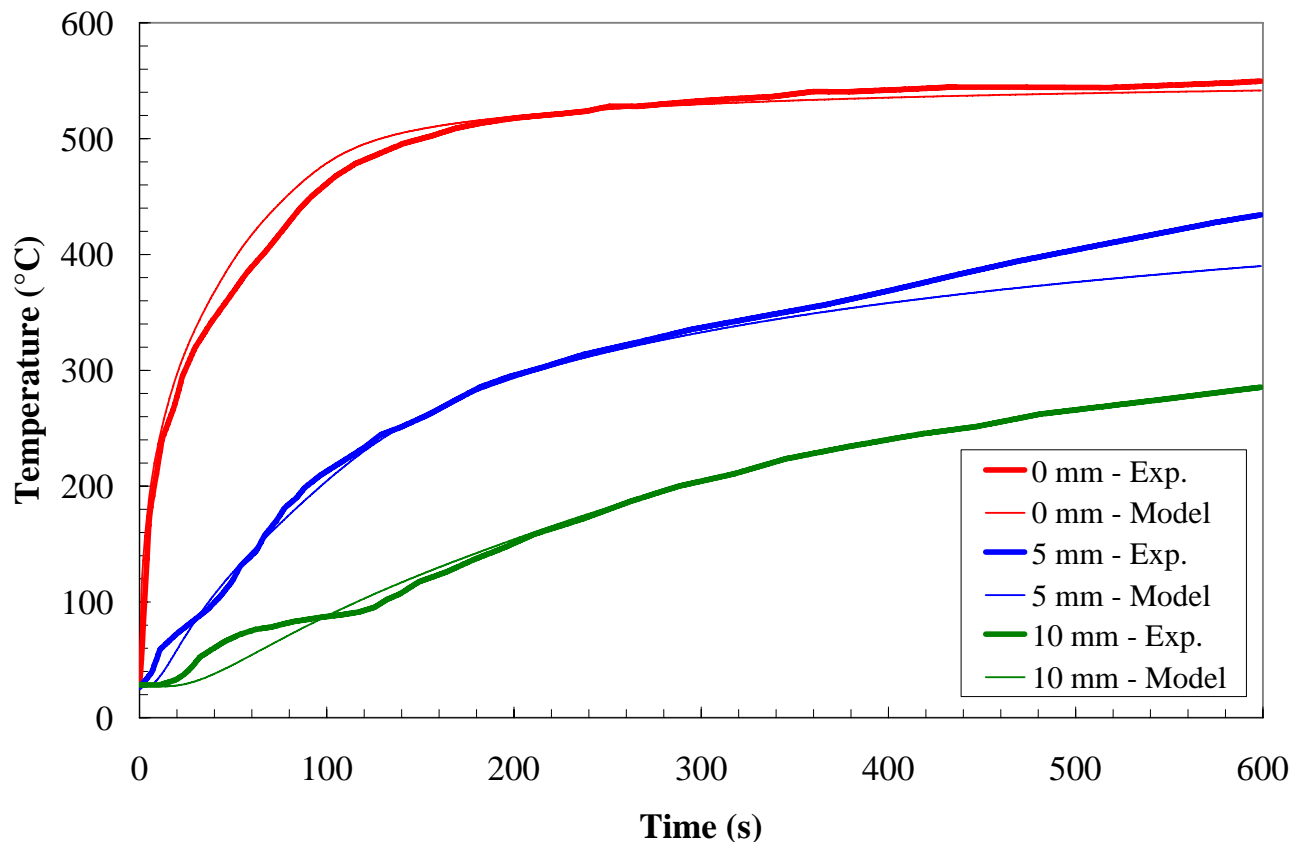
- Modeling approach
 - 4 solid species: wet wood, dry wood, char, ash
 - 4 solid reactions: drying, dry wood pyrolysis, dry wood oxidation, char oxidation
 - 1 gas-phase reaction: oxidation of pyrolysate
 - 5 gaseous species: N_2 , O_2 , H_2O , pyrolysate, products
- The challenge
 - At least 40 unknown model parameters must be specified!
- The solution
 - Parameters estimated from experimentally measured MLR and T using genetic algorithm-based optimization



White Pine – Comparison of Measured and Modeled T



- Modeled temperatures match experimental data quite well for pyrolysis under N_2 :

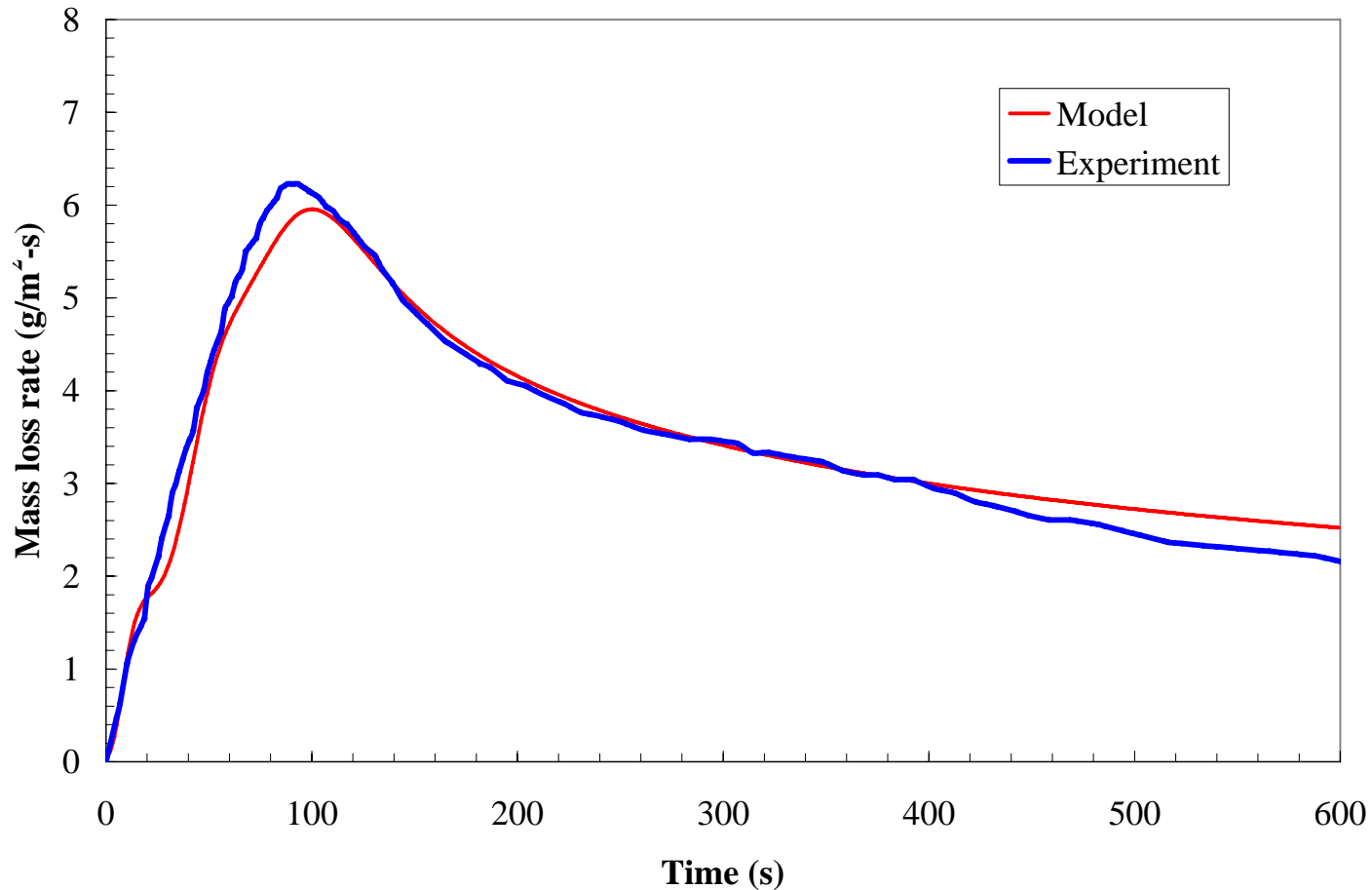




White Pine Oxidative Pyrolysis – Predictions/Measurements in N_2



- Mass loss rate under N_2 :

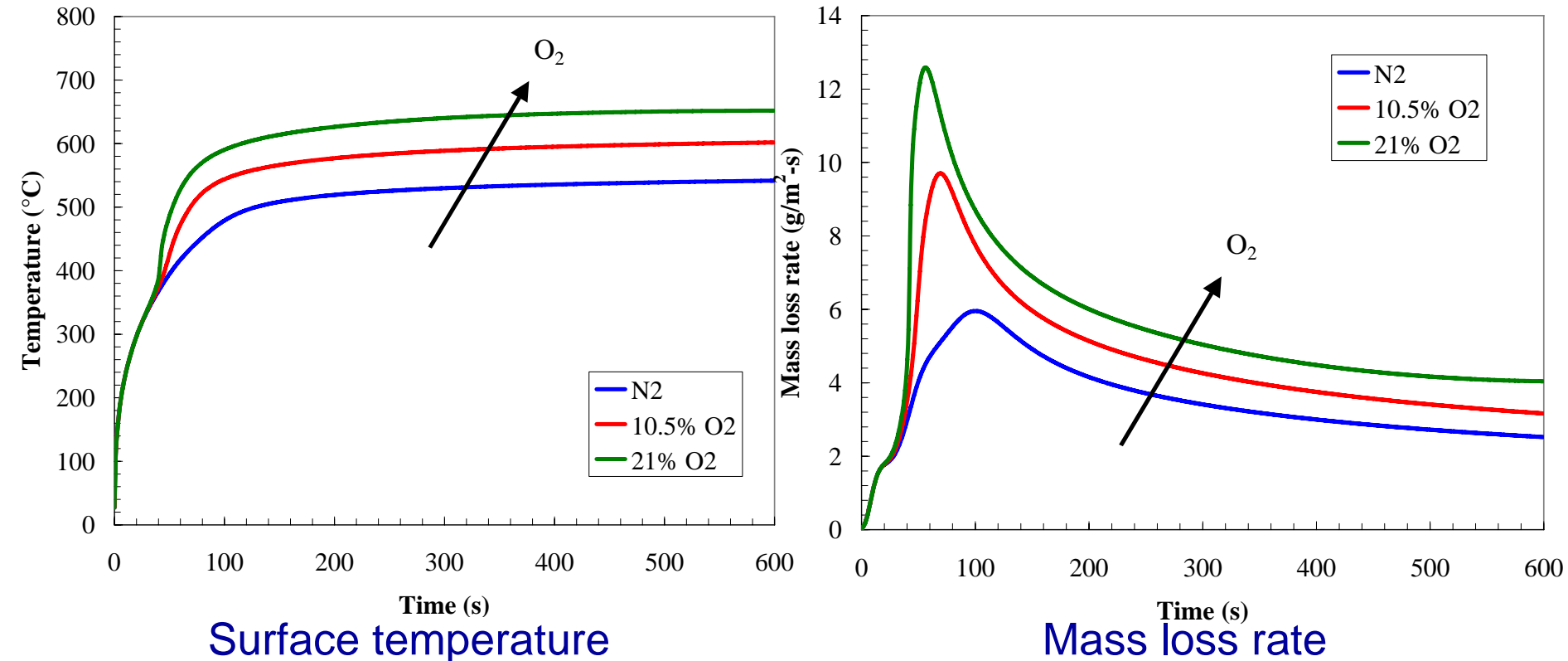




White Pine Oxidative Pyrolysis – Model Predictions



- Model captures experimentally-observed increase in MLR and surface T with increasing O_2 concentration

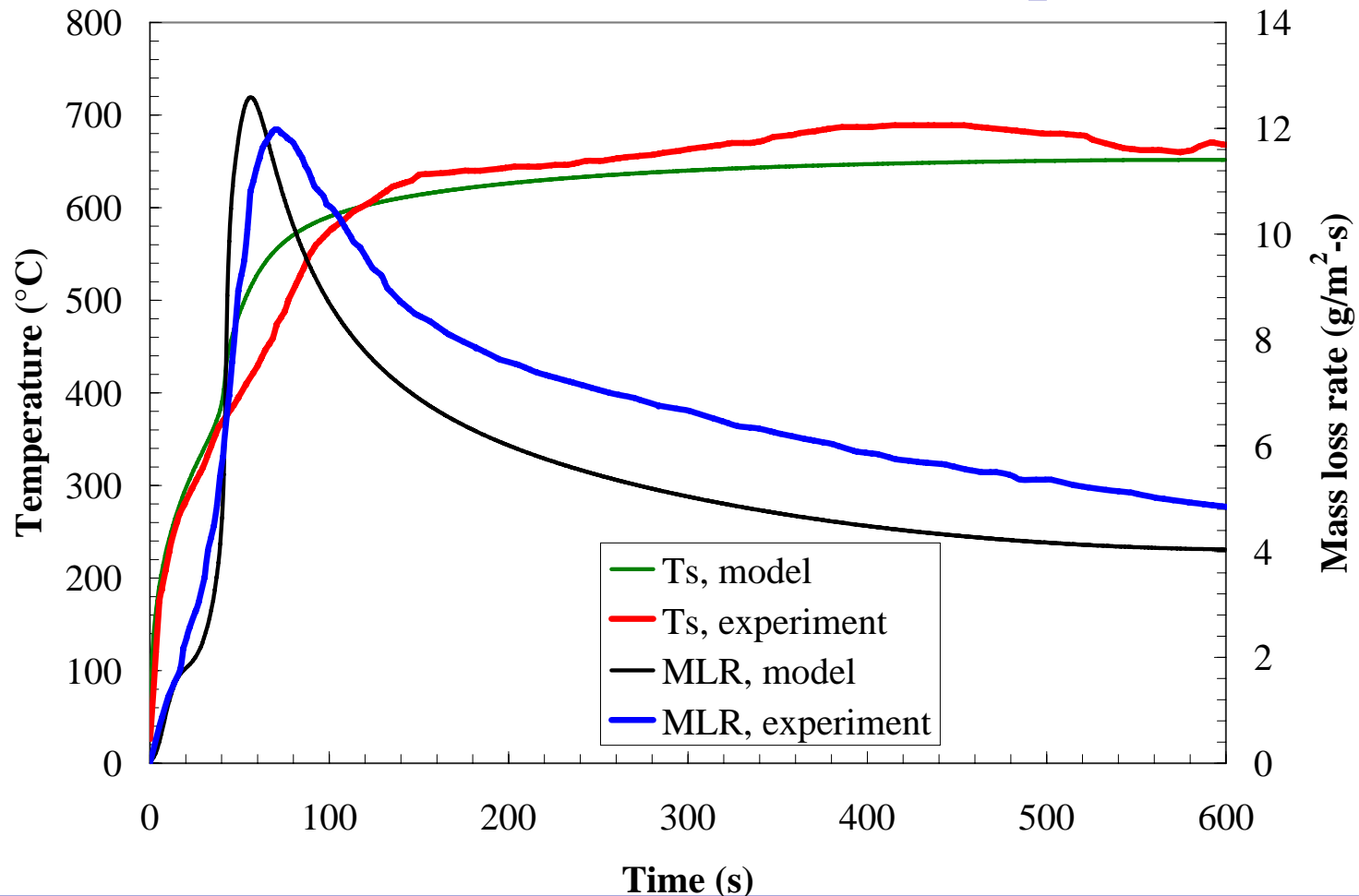




White Pine Oxidative Pyrolysis – Predictions/Measurements in Air

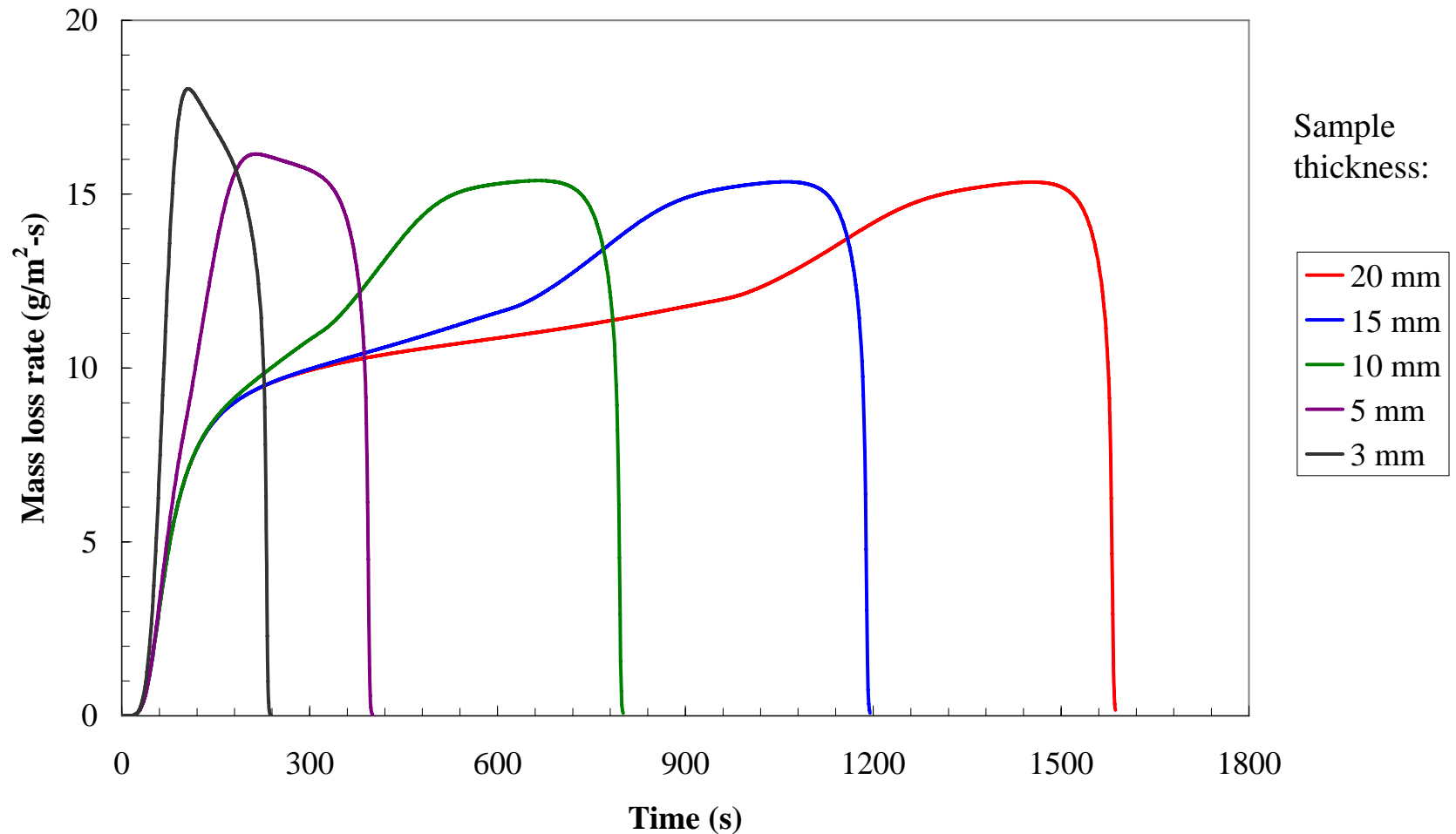


- Surface temperature and MLR (21% O₂)





Polypropylene Pyrolysis – Effect of Thickness





Heating and Swelling of an Intumescent Coating

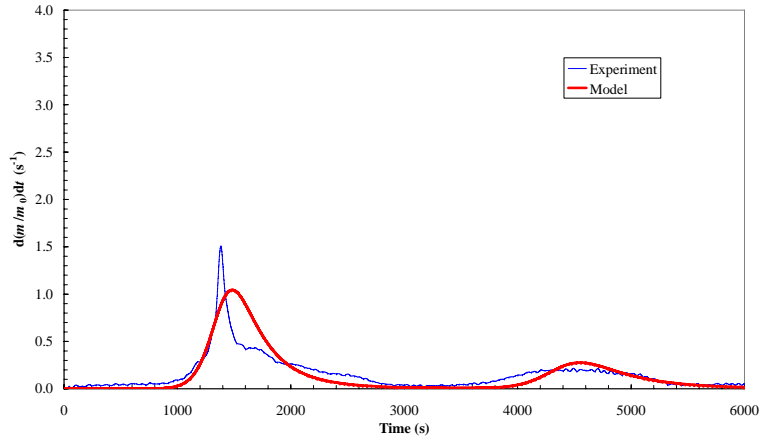


- Experiment - Griffin *et al.*, *JFS* v23 (2005)
 - Cone Calorimeter
 - 2.7 mm intumescent coating applied over steel substrate
 - Irradiated at 90 kW/m² (T_{subs} and δ measured)
 - Thermogravimetric analysis (TGA)

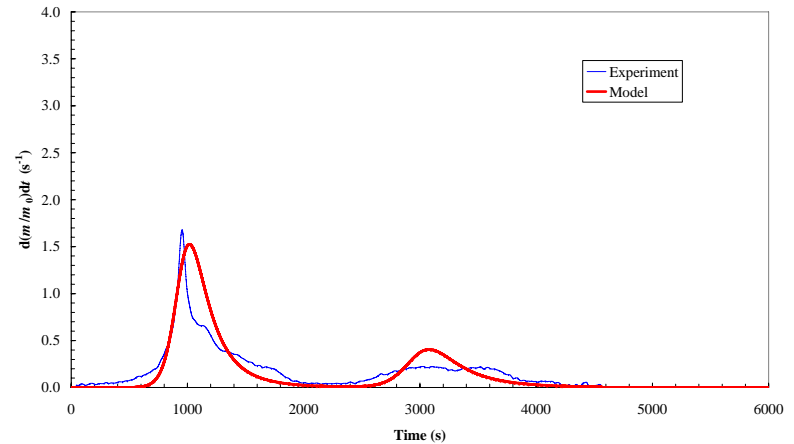
- Modeling approach
 - 5 solid species
 - 3 condensed-phase reactions, including intumescence
 - 26 model parameters determined by genetic algorithm optimization



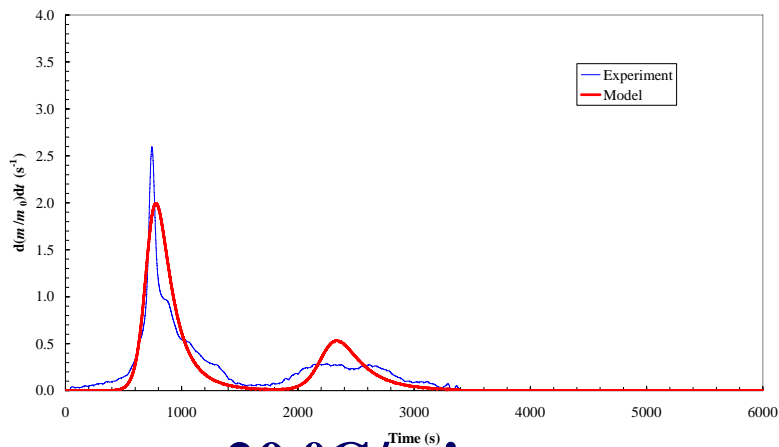
Intumescent Coating – Model Results (TGA)



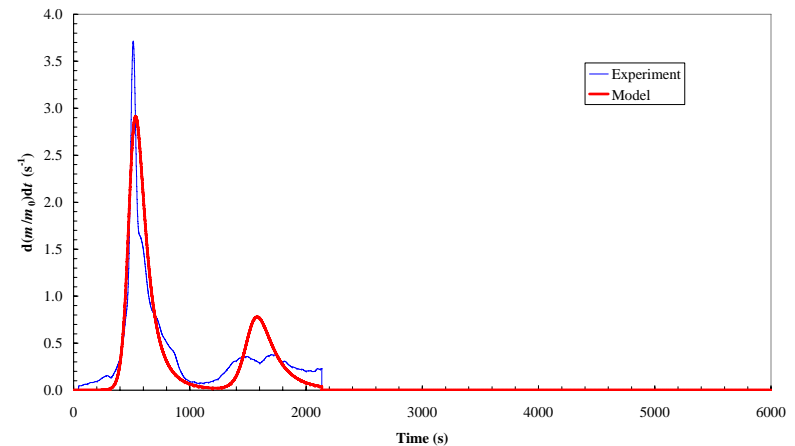
10 °C/min



15 °C/min



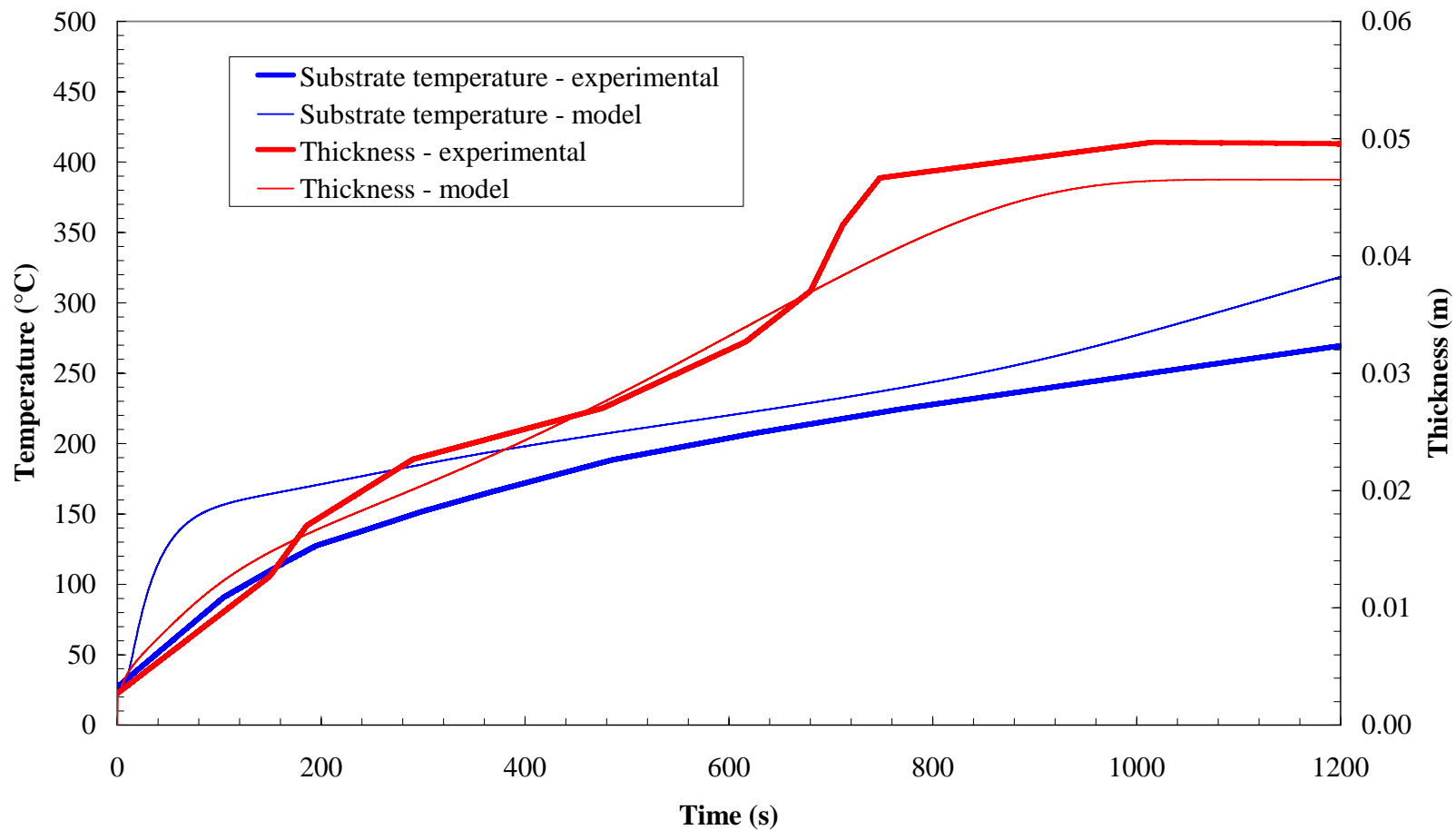
20 °C/min



30 °C/min



Intumescent Coating – Model Results (Cone Calorimeter)





Concluding Remarks



- Pyrolysis model simulates well multiple materials
- Material property estimation via genetic algorithm optimization seems to “work” even for search spaces with 20+ adjustable parameters
- Future work
 - Additional materials (composites, charring polymers)
 - Extension to 2D (anisotropy, transition to flaming)
 - Predicting real world flame spread and fire growth via coupling to CFD code